NTNU – Trondheim
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Department of Physics

Examination paper for FY2045 Quantum Mechanics I

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15:00-19:00

Part I ($\sim 30\%$)

Answer the following questions in Inspera.

Problem 1 Multiple choice problems

Choose only **one** of the options for each problem.

a) Consider a system of two non-interacting particles. The first particle is in an eigenstate of its operator for the square of the total angular momentum, $\mathbf{J}_1^2$,

$$\mathbf{J}_1^2|j_1, m_1\rangle = \hbar^2 j_1(j_1+1)|j_1, m_1\rangle,$$

with $j_1 = 5$. The second particle is in an eigenstate of its operator for the square of the total angular momentum, $\mathbf{J}_2^2$,

$$\mathbf{J}_2^2|j_2, m_2\rangle = \hbar^2 j_2(j_2+1)|j_2, m_2\rangle,$$

with $j_2 = 2$. The possible values of the square of the total angular momentum operator of the two-particle system are given by

$$\hbar^2 j(j+1).$$

What are the possible values of j?

A $j = 0, 1, \ldots, 5$
B $j = 2, 3, 4, 5$
C $j = 3, 4, 5, 6, 7$
D $j = -7, -6 \ldots, 6, 7$
E $j = 0, 1, \ldots, 7$

b) What is the normalized eigenspinor of $S_x = \frac{\hbar}{2}\sigma_x$ corresponding to the eigenvalue $+\frac{\hbar}{2}$?

A $\chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

B $\chi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

C $\chi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$

D $\chi = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

E $\chi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

c) Which of the following spin states for a spin $\frac{1}{2}$ particle gives a probability of 0.9 of getting the value $\hbar/2$ when measuring the spin along the x direction?

A $\chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

B $\chi = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ 1 \end{pmatrix}$

C $\chi = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ -i \end{pmatrix}$

D $\chi = \frac{1}{\sqrt{10}} \begin{pmatrix} 3 \\ 1 \end{pmatrix}$

E $\chi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

d) At time $t = 0$, a particle with spin $\frac{1}{2}$ is measured to be in the spin state

$$\chi(t = 0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{1}$$

a superposition of the energy eigenstates of the system Hamiltonian,

$$H = \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2}$$

What is $\chi(t)$, that is, the spin state of the particle at time $t \geq 0$?

A $\chi(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

B $\chi(t) = \begin{pmatrix} e^{-i\omega t} \\ 0 \end{pmatrix}$

C $\chi(t) = \begin{pmatrix} 0 \\ e^{i\omega t} \end{pmatrix}$

D $\chi(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix}$

E $\chi(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega t} \\ e^{-i\omega t} \end{pmatrix}$

e) Again, consider the particle described by the Hamiltonian in Eq. (2), measured to be in the spin state in Eq. (1) at $t = 0$. Assuming no measurements have been made since $t = 0$, which of the following statements is true?

A If you measure the spin along x, you will always get $S_x = \hbar/2$.
B At $t = \frac{\pi}{2\omega}$ you are guaranteed to measure $S_y = -\hbar/2$.
C It is always impossible to know the outcome of a measurement of S_y.
D At $t = \frac{\pi}{2\omega}$ you are guaranteed to measure $S_x = -\hbar/2$.
E If you measure the energy of the particle, you lose all information about the spin state of the particle.

f) In the general formulation of quantum mechanics, the momentum representation is found by considering eigenstates of the momentum operator $\hat{p}$, defined by

$$\hat{p}|p\rangle = p|p\rangle,$$

where p is an eigenvalue. What is $\langle p_2|\hat{p}|p_1\rangle$?

A $p_2\delta(p_2 - p_1)$
B $\frac{\hbar}{i}\frac{\partial}{\partial p_1}\delta(p_2 - p_1)$
C $\delta(p_2 - p_1)$
D 0
E $-\frac{\hbar}{i}\frac{\partial}{\partial x}\delta(p_2 - p_1)$

g) A particle is described by a wave-packet

$$\Psi(x,t) = \langle x|\Psi\rangle = \int_{-\infty}^{\infty} \phi(k) e^{i[kx-\omega(k)t]} dk, \tag{3}$$

where $\omega(k) = \hbar k^2/(2m)$, and m is the mass of the particle. The coefficients $\phi(k)$ have a distribution

$$\phi(k) = \sqrt{\frac{1}{2\sigma\pi^{3/2}}} e^{-(k-k_0)^2/(2\sigma^2)}, \tag{4}$$

where the constant σ is real and larger than 0. The distribution has a large and narrow peak at $k = k_0$, with a finite width. What is momentum-space wavefunction $\Phi(p,t) = \langle p|\Psi\rangle$ corresponding to the wave-packet in Eqs. (3) and (4)? *The following might be useful:* $\psi_p(x) = \langle x|p\rangle = (2\pi\hbar)^{-1/2} e^{ipx/\hbar}$.

A $\Phi(p,t) = \phi(p)$

B $\Phi(p,t) = \sqrt{2\pi/\hbar}\,\phi(p/\hbar)e^{-ip^2t/(2m\hbar)}$

C $\Phi(p,t) = \phi(p/\hbar)e^{-ip^2t/(2m\hbar)}$

D $\Phi(p,t) = \phi(p/\hbar)$

E $\Phi(p,t) = \sqrt{2\pi\hbar}\,\phi(p/\hbar)e^{-ip^2t/(2m\hbar)}$

h) A particle is in the state

$$|\psi\rangle = \sqrt{\frac{2}{6}}|1\rangle + \sqrt{\frac{4}{6}}|2\rangle,$$

where $|1\rangle$ and $|2\rangle$ are energy eigenstates with energies $E_1 = \hbar\omega$ and $E_2 = 2\hbar\omega$, respectively. What is the expectation value of the energy for the state $|\psi\rangle$?

A $\langle E\rangle = \frac{3\hbar\omega}{2}$

B $\langle E\rangle = \hbar\omega$

C $\langle E\rangle = \frac{4\hbar\omega}{3}$

D $\langle E\rangle = 2\hbar\omega$

E $\langle E\rangle = \frac{5\hbar\omega}{3}$

i) Consider the normalized state vector

$$|\psi\rangle = \frac{1}{\sqrt{6}}\left[(2+i)|1\rangle + i|2\rangle\right],$$

where $|1\rangle$ and $|2\rangle$ are orthonormal basis vectors. What is $\langle\psi|$, the dual vector of $|\psi\rangle$?

A $\langle\psi| = \frac{1}{\sqrt{6}}\left[(2+i)|1\rangle + i|2\rangle\right]$

B $\langle\psi| = \frac{1}{\sqrt{6}}\left[\langle 1| + \langle 2|\right]$

C $\langle\psi| = \frac{1}{\sqrt{6}}\left[(2-i)\langle 1| - i\langle 2|\right]$

D $\langle\psi| = \frac{1}{\sqrt{6}}\left[(2+i)\langle 1| + i\langle 2|\right]$

E $\langle\psi| = \frac{1}{\sqrt{6}}\left[(2-i)\langle 1| + i\langle 2|\right]$

Problem 2 Short answer questions

Give a short answer (maximum 2-3 sentences) to **two of the three** questions below. You may use simple equations in your answer.

a) What are the main differences between fermions and bosons?

b) What is the Pauli exclusion principle, and what is the reason behind it?

c) Why do physical observables have to be represented by Hermitian operators?

Part II $(\sim 70\%)$

Write your calculations and answers to the following problems on paper. Clearly mark each page and answer with the problem number.

Problem 3

Consider a three-dimensional box with lengths $L_x = L_y = L$ and L_z, where the potential is zero inside and infinite outside.

a) Show why the stationary state wavefunctions take the form

$$\psi_{n_x n_y n_z} = A \sin\frac{\pi x n_x}{L} \sin\frac{\pi y n_y}{L} \sin\frac{\pi z n_z}{L_z},\ (0 < x < L,\ 0 < y < L,\ 0 < z < L_z), \tag{5}$$

where n_x, n_y, n_z are positive integers, and that the one-particle energies are given by

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2 + n_y^2}{L^2} + \frac{n_z^2}{L_z^2} \right), \tag{6}$$

where m is the mass of the particle in the box.

b) We place 22 identical non-interacting fermions with spin 1/2 in the box. With $L_z = 0.1L$, what is the maximal occupied one-particle energy $E_{n_x n_y n_z}$ when the system is in the ground state, that is, the total system energy is as low as possible?

c) Calculate $N(E)$, the total number of single-particle states with energy less than E in the macroscopic limit (L large) when all sides of the box are equal, $L_x = L_y = L_z = L$. Use the result to calculate the density of states, $g(E)$.

Problem 4

Derive the equation

$$\frac{d}{dt}\langle F \rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{F}] \rangle + \left\langle \frac{\partial \hat{F}}{\partial t} \right\rangle \tag{7}$$

using the general definition of an expectation value in the state $|\psi\rangle$,

$$\langle F \rangle = \langle \psi | \hat{F} | \psi \rangle. \tag{8}$$

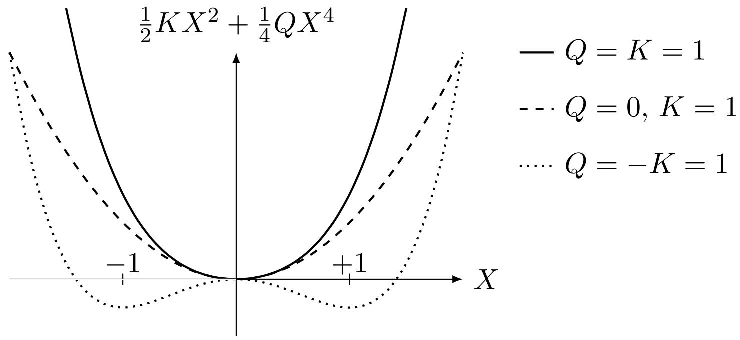
You are free to use any formulation of quantum mechanics. *Hint:* Use the product rule.

Problem 5

Consider a system described by the Hamiltonian

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}k\hat{x}^2 + \frac{1}{4}q\hat{x}^4, \tag{9}$$

where k and q are real parameters, with $q \geq 0$. A sketch of the potential using dimensionless quantities is shown below.



When $q = 0$ and $k > 0$, Eq. (9) describes a harmonic oscillator, and the Schrödinger equation can be solved by introducing the ladder operators

$$\begin{aligned} a &= \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{x} + \frac{i}{m\omega}\hat{p}_x\right], \\ a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{x} - \frac{i}{m\omega}\hat{p}_x\right], \end{aligned} \tag{10}$$

with $\omega \equiv \sqrt{k/m}$. The resulting energies are

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right),\ (n = 0, 1, 2\ldots), \tag{11}$$

with orthonormal eigenstates $|n\rangle$ defined by the eigenvalue equation

$$a^\dagger a|n\rangle = n|n\rangle, \tag{12}$$

and

$$a|0\rangle = 0. \tag{13}$$

a) Use Eqs. (10) and (13) to show that the position space wavefunction $\psi_0(x)$ of the ground state of the harmonic oscillator is

$$\psi_0(x) = Ae^{-m\omega x^2/2\hbar}. \tag{14}$$

Hint: The following might be useful:

$$\langle x|n\rangle = \psi_n(x),$$
$$1 = \int dx\ |x\rangle\langle x|,$$
$$\langle x''|F(\hat{x},\hat{p}_x)|x'\rangle = F\left(x'', \frac{\hbar}{i}\frac{\partial}{\partial x''}\right)\delta(x''-x').$$

Some of the integration formulas given in the formula sheet might also be useful for this problem.

b) Calculate the normalization constant A in Eq. (14).

c) We now assume $k>0$ and $q>0$ and treat the last term in Eq. (9) as a perturbation, $\hat{V}_q = \frac{1}{4}q\hat{x}^4$. Given the following properties of the raising and lowering operators in Eq. (10),

$$a|n\rangle = \sqrt{n}|n-1\rangle,$$
$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle,$$

calculate the first-order corrections to the energies using

$$E_n^{(1)} = \langle n|\hat{V}|n\rangle. \tag{17}$$

Briefly comment on the result.

Hint: Since the eigenstates $|n\rangle$ are orthonormal, $\langle m|n\rangle = \delta_{nm}$, expectation values containing unequal numbers of raising and lowering operators are zero, e.g. $\langle n|aa^\dagger aa|n\rangle = 0$ etc.

d) When $k<0$ and $q>0$ we cannot use perturbation theory based on the states $|n\rangle$ and corresponding energies in Eq. (11) — why?

e) Calculate the expectation value of the energy, $\langle H\rangle$, when $k<0$ and $q>0$ using the trial function

$$\psi_c(x) = Ce^{-m\Omega(x-x_0)^2/2\hbar}, \tag{18}$$

where $\Omega = \sqrt{-2k/m}$ and x_0 is a free parameter. *Hint:* It can be useful to shift the integration variables

$$\int_{-\infty}^{\infty} dx\ x^{2n}e^{-a(x-x_0)^2} = \int_{-\infty}^{\infty} dx\ (x+x_0)^{2n}e^{-ax^2}, \tag{19}$$

and keep in mind that e^{-ax^2} is an even function of x.

f) Use the variational method to find an upper bound for the ground state energy. To simplify the calculations, you can consider the limit $\hbar\Omega q/k^2 \ll 1$ and keep leading order terms in $\hbar\Omega$. Do the results for the upper bound and x_0 seem reasonable?

A Formula sheet

Schrödinger equation (time-dependent and time-independent)

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$$
$$\hat{H}|\psi\rangle = E|\psi\rangle$$

Thermodynamics

$$dW = PdV$$

Eigenvalues and eigenvectors

$$\det(A - \lambda I) = 0$$
$$(A - \lambda I)\mathbf{v} = 0$$

Some properties of the Dirac delta function and Heaviside step function

$$\int dx\ f(x)\delta(x-a) = f(a)$$
$$\frac{1}{2\pi}\int dx\ e^{i(k-k_0)x} = \delta(k-k_0)$$
$$\Theta(x) = \begin{cases} 1, & x > 0, \\ 0, & x \leq 0. \end{cases}$$
$$\frac{d}{dx}\Theta(x) = \delta(x)$$
$$\int_{-\infty}^{\infty} dx\ \left[\frac{d}{dx}\delta(x)\right] f(x) = -\int_{-\infty}^{\infty} dx\ \delta(x)\left[\frac{d}{dx}f(x)\right]$$

Various physical constants

$$\hbar = 1.054\,571\,817 \times 10^{-34}\,\mathrm{J\,s} = 6.582\,119\,569 \times 10^{-16}\,\mathrm{eV\,s}$$
$$m_e = 9.109\,383\,701\,5 \times 10^{-31}\,\mathrm{kg}$$
$$e = 1.602\,176\,634 \times 10^{-19}\,\mathrm{C}$$
$$c = 299\,792\,458\,\mathrm{m\,s^{-1}} \approx 3 \times 10^{8}\,\mathrm{m\,s^{-1}}$$
$$\mu_0 = \frac{1}{\epsilon_0 c^2} = \frac{4\pi\alpha}{e^2}\frac{\hbar}{c} = 1.256\,637\,062\,12 \times 10^{-6}\,\mathrm{N\,A^{-2}}$$
$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137}$$
$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{e^2 m_e} = 5.29 \times 10^{-11}\,\mathrm{m}$$

$$\mu_B = \frac{\hbar e}{2m_e} = 9.274\,010\,078\,3 \times 10^{-24}\,\mathrm{J\,T^{-1}} = 5.788\,381\,806\,0 \times 10^{-5}\,\mathrm{eV\,T^{-1}},$$

Commutators and anticommutators

$$\begin{aligned}
[A, B] &\equiv AB - BC \\
[AB, C] &= [A, C]B + A[B, C] \\
[A + B, C] &= [A, C] + [B, C] \\
\{A, B\} &\equiv AB + BA
\end{aligned}$$

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Taylor expansion

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dx}\right)^n f(x)\bigg|_{x=a} (x-a)^n$$

Some potentially useful integrals

$$\begin{aligned}
\int_{-\infty}^{\infty} dx\ e^{-a(x+b)^2} &= \sqrt{\frac{\pi}{a}} \\
\int_{-\infty}^{\infty} dx\ e^{-ax^2+bx+c} &= \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}+c} \\
\int_{-\infty}^{\infty} dx\ x^{2n} e^{-ax^2} &= \left(-\frac{\partial}{\partial a}\right)^n \int_{-\infty}^{\infty} dx\ e^{-ax^2}
\end{aligned}$$

Cylindrical coordinates

$$\begin{aligned}
x = r\cos\phi, \quad y &= r\sin\phi, \quad z = z \\
\boldsymbol{\nabla} f &= \frac{\partial f}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial f}{\partial \phi}\hat{\phi} + \frac{\partial f}{\partial z}\hat{z} \\
\boldsymbol{\nabla} \cdot \mathbf{A} &= \frac{1}{r}\frac{\partial}{\partial r}(rA_r) + \frac{1}{r}\frac{\partial A_\phi}{\partial \phi} + \frac{\partial A_z}{\partial z} \\
\nabla^2 f &= \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2} \\
\int d\mathbf{r} &= \int dz\ d\phi\ dr\ r
\end{aligned}$$

Spherical coordinates

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta$$

$$\boldsymbol{\nabla} f = \frac{\partial f}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\hat{\phi}$$

$$\boldsymbol{\nabla}\cdot\mathbf{A} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 A_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}\left(A_\theta \sin\theta\right) + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial \phi}$$

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial \phi^2}$$

$$\int d\mathbf{r} = \int d\phi\ d\theta\ dr\ \ \sin\theta r^2$$